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# Simulation of X-Ray Diffraction Data of Cr-Doped $Mn_2NiSn$ System Quaternary Heusler Alloys

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**Abstract.** Quaternary Heusler alloys have attracted considerable attention due to their structural versatility, tunable magnetic properties, and potential for spintronic applications. Here, we have simulated the X-Ray Diffraction data for systematic substitution of the $Mn_{2-x}Ni_{1-x}Cr_{2x}Sn$ system ($0 \leq x \leq 1.0$) alloy where substitution of Cr at Ni and Mn site has been employed in $Mn_2NiSn$ parent cubic structure. Structural analysis through simulated X-ray Diffraction data obtained from Vesta have performed from the ratio of super reflection peaks associated with the cubic phase. Although, XRD data is not reliable for the analysis of swapping of substituted atoms due the equivalent atomic size and electro-negativity between them. Neutron diffraction technique is best suitable for the exact analysis of occupation of elements at their respective site. However, we have found a significant change in the intensity of simulated XRD pattern and hence focused on the highly sensitive peaks. Magnetic properties of these materials have been found to be strongly correlated with the structure, substitution, doping, swapping of elements. Hence, we have particularly focused on the Cr substitution at both Mn and Ni site and noted the change in the intensities of super reflection peaks. Experimental work is currently going on these materials also.

## 1 Introduction

Heusler alloys have been traced as a potential material due to their wide magnetic behavior even at room temperature. Among the other, Co and Mn based Heusler alloy have revealed the highest magnetic moment and found to be easily fabricated in pure structure. Half and full-Heusler (FH) are almost similar excepted one vacant site is present in half-Heusler (HH). Atomic sites are given by XI (0, 0, 0), XII (½, ½, ½,), Y (¼, ¼, ¼) and Z (¾, ¾, ¾) in both the case with missing of XII in HH. Several Heusler's such as $Mn_2NiSn$ and $Mn_2NiSb$ in $Mn_2$-based and $Co_2MnSi$ and $Co_2FeSi$ in $Co_2$-based family have been exhibited to be a most favorable alloys in comparison to others [1-5]. Substitution of other elements have implemented in the parent structure and found the significant tuning in their magnetic

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properties. These substitution changes the relative intensities of superlattice reflections (111 and 200) and ratio of both gives the significant information about the minor change in atomic swapping/substitution. In order to identify the effect of substitution, experimental data should be matched with the calculated one through the Rietveld refinement. Although, standard crystallographic information file (cif) would be needed to perform the refinement process. Hence, cif could be generated from Vesta and used for the matching of both the data.
Here, we have substituted the Cr at Mn and Ni site in $Mn_2NiSn$ with almost all possible combination ranges from 0-100% substitution. Generally, Cr have been showed an antiferromagnetism in their ground state structure and might be aligned parallel in $Mn_2NiSn$. Therefore, we have intensively chosen the Cr for the replacement and noted the ratio ($\alpha$) for each nominal substitution. Several reports on Cr doping have reported such as Cr doping in NiMnSb, NiCoMnSn, NiMnGa, $Co_2FeAl$, $Co_2FeSi$, $Mn_2NiGa$ etc. Substitution of Cr at Mn site in NiMnSb, ferromagnetism has been found to be increased while exchange biasing and magnetoresistance suppressed with the destabilization of martensitic phase [6]. Mechanical properties have been found to be notably increased with Cr doping in NiCoMnSn due to the reduced martensite phase with the evolution of $\gamma$-eutectic phase [7]. Cr doped NiMnGa have showed the magnetic entropy change in the system [8]. In $Co_2Fe_{0.4}Cr_{0.6}Al$, magnetic moment has enhanced in comparison to metallic phase of Cr and moment of Co has also increased in comparison to bulk [9]. Moreover, Cr substituted at Fe site in $Co_2FeSi$ from 2-10% have performed and found the highest spin polarization at 2% and constant up to 4% [10]. In $Mn_2NiGa_{1-X}Cr_X$, coexistence of BCC and FCC phase was observed at x = 0.375 and pure FCC was revealed at x=0.5 while saturation magnetization has found to be increased for FCC phase due to the parallel alignment of moment of Cr with Mn moment [11].

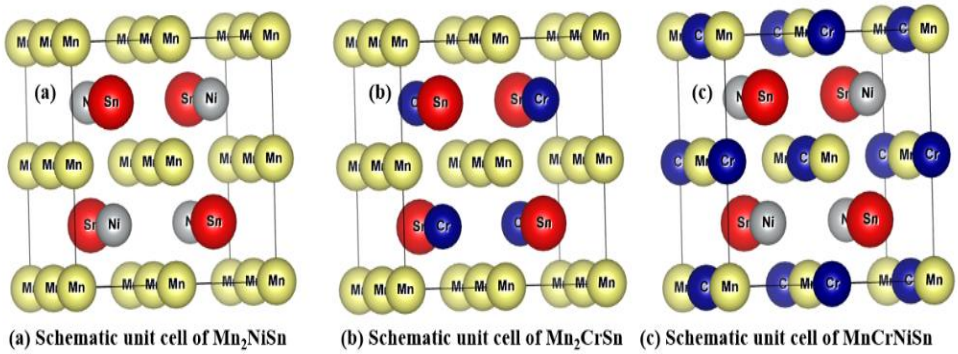


**Fig. 1** Schematic Unit cell of $Mn_2NiSn$, $Mn_2CrSn$ and MnCrNiSn half and full-Heusler alloys.

All the studies suggests that crystallographic parameters are drastically changed which in turn tuned the physical properties of the sample. From this motivation, we have elaborated the XRD data obtained from the Vesta for Cr substitution in $Mn_2NiSn$ i.e. $Mn_{2-X}Ni_{1-X}Cr_{2X}Sn$ ($0 \leq X \leq 1$).

## 2 Method

Vesta software is used to obtain the XRD pattern of each partially and fully Cr-substituted at Mn (I), Mn (II) and Ni site in $Mn_2NiSb$ full-Heusler alloy via different occupation numbers. First two super-reflection peaks in each pattern have been rigorously analyzed due the its highly sensitivity for exchanging, substituting or doping the other elements. Origin software has used to plot the data between the concentration and ratio of 111 and 200.

## 3 Results and Discussions

Intensity ratio ($\alpha$) of super reflections peaks have been eliminated from the simulated XRD data through Vesta for Cr-substituted $Mn_2NiSn$ full-Heusler. Cr has substituted at Mn (I), Mn (II) and Ni site in different condition. Since, scattering amplitude of Cr has found to be lesser from Mn so the intensity should be increased for the planes containing more Cr atoms or having much occupancy of Cr atoms. From the Fig. 2, we can see that $\alpha$ has increased with the Cr concentration at Ni site more rapidly than others due to the more scattering factor of Cr than Ni. Lowest value of $\alpha$ has been found for Cr substitution at Mn (0.5, 0.5, 0.5) site and all the values lie between the partial substitution at Ni and Mn substitution simultaneously, and at Mn (0, 0, 0) site separately. The rate of enhancement of $\alpha$ value for Cr substituted at Mn (0.5, 0.5, 0.5) with negative slope have changed less rapidly in accordance with the rate of enhancement of curve for Cr substituted at Ni site. This is obvious due to the scattering amplitude of Cr lying between Ni and Mn. Although, different planes have contained different elements so the effective number of particular atoms in any specific plane also matters. Hence, we have obtained different slopes for Cr substitution at Mn (0, 0, 0) and Mn (0.5, 0.5, 0.5) sites because different occupancy of Mn have revealed in 111 and 200 planes.

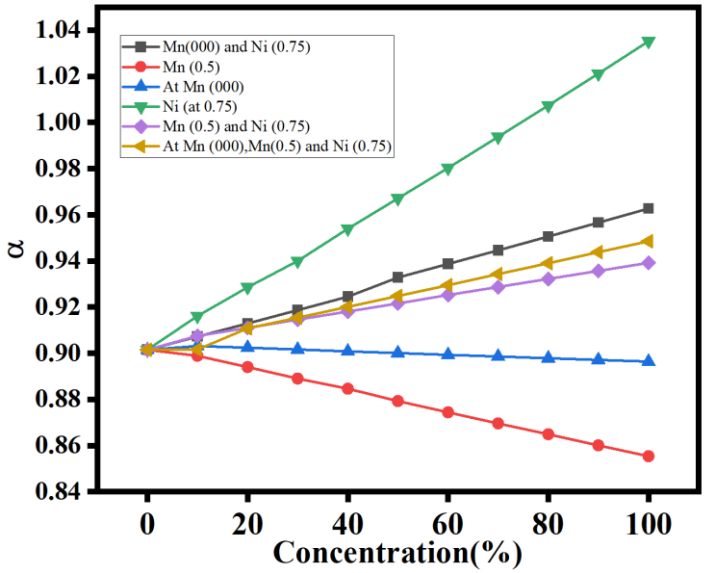


**Fig. 2** Curve between the $\alpha$ (ratio of 111 and 200 planes) versus concentration of Cr at different site in $Mn_2NiSn$.

Scattering amplitude of Cr, Ni, Mn and Sn have plotted in the Fig. 3 for the sake of simplicity in order to understand the plotted data in Fig. 2.

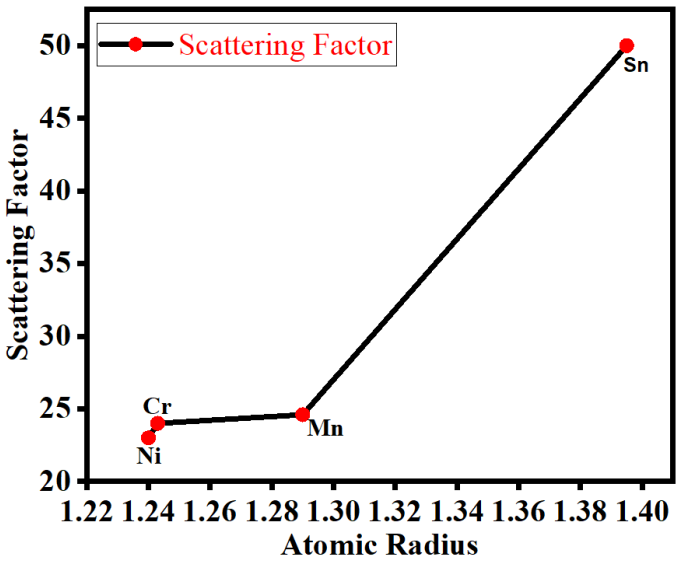


**Fig. 3** Curve between Atomic radius versus scattering factor taken from NIST

Moreover, we have not made any changes with the Sn elements in FCC structure and therefore corresponding data have not considered here. However, effect of exchange interaction relatively affects the Sn atoms also and subsequently, scattering amplitude will be changed accordingly.

## 4 Conclusion

Cr substitution of $Mn_2NiSn$ have successfully implemented through Vesta. Ratio of super reflection peaks have plotted with concentration of Cr at different sites individually and simultaneously which suggested the enhancement of $\alpha$ with Ni replacement, reduction of $\alpha$ with Mn replacement etc. The slopes of all the curves have been explained on the basis of scattering factors data taken from the NIST, USA. Partial substitution of Cr has been theoretically implemented through the occupancy factor given in the vesta. These analyses are fruitful for the material's researcher for the comparison of XRD data in order to assure the definite site preference of the elements.

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